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Ab-inito calculation of energy level alignment and vacuum level shift at CuPc/C60 interfaces[1] NA SAI, XIAOYANG ZHU, JAMES CHELIKOWSKY, University of Texas at Austin, KEVIN LEUNG, Sandia National Laboratory — The alignment of the donor and acceptor enegy levels is of crucial importance for organic photovotaic performance. We investigate the interfaical electronic structure and energy level alignment of copper phthalocyanine (CuPc)/fullerene (C60) using ab-inito density functional theory calculations including van der Waals interactions and hybrid density functionals. We show that energy level alignment critically depends on the standing-up and lying-down orientation of the CuPc molecules relative to C60 at the interface. We calculate the magnitude of the interface dipole at different molecular orientations and compare them to the vacuum level shift observed in photoemission spectroscopy. The validity of existing theoretical models which invoke charge transfer on this organic interface will be discussed in light of our predictions. Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Deparment of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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